RESEARCH HIGHLIGHTS

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I. INTRODUCTION

Large Eddy Simulation (LES) is a numerical simulation technique that has became very popular in the last two decades. It is based on separate simulation of large-scale and small-scale features of the fluid flow; the large scales are directly computed from numerical scheme and the effect of small scales is modeled via *subgrid-scale (SGS) models*.

The separation between large and small scales is formally performed by applying a low-pass filter to the governing equations of motion. In particular case of Navier-Stokes equations, the nonlinear term gives rise to the unclosed term in the new LES equations of motion. Modeling these terms is the central subject of LES.

Although it may appear that the small-scale features of the flow do not play an important role in the large-scale dynamics, more and more recent studies show that the quality of the representation of the effect of SGS scales is crucial for the quality of simulation.

There are two kinds of tests that can be administered on a proposed SGS model:

- *A priori* test. In this test, a fully resolved (without any modeling) flow field is used, obtained either from Direct Numerical Simulation (DNS) or from experimental measurements. The flow field is filtered and the SGS terms are calculated directly. Then the filtered flow field is used to evaluate the proposed model, and then the model is compared to the true SGS term.

- *A posteriori* test. In this test, the models are incorporates into the computer program and the outcome of the simulation is compared to the data available from elsewhere, e.g., to averaged DNS data or to experimental measurement.

The former requires the database of results of DNS of canonical flows such as homogeneous isotropic turbulence, where the model effects can be isolated and studied. The latter requires an LES code.

II. HIGH-RESOLUTION DNS DATABASE

A cutting-edge DNS database is currently under construction. The resources used are Coyote and QSC supercomputers at LANL. The database contains snapshots of velocity and scalar fields from simulations of decaying and forced isotropic homogeneous turbulence with various resolutions: 256^3, 512^3 and 1024^3 points. Extension to 2048^3 run is possible. The highest resolution currently reported in the literature is 4096^3 grid points.

To verify that the simulations have fully developed range of scales, we check the well-known Kolmogorov 4/5-rule: $S_3(r) \equiv \langle(\delta u)^3\rangle = -\frac{4}{5}\langle\epsilon\rangle r$, where S_3 is the third-order structure function. The scaling of S_3 is presented in the Figure 1; a snapshot from a 1024^3 simulation is shown in Figure 2. It should be noted that the 1024^3 simulation is not fully developed yet.

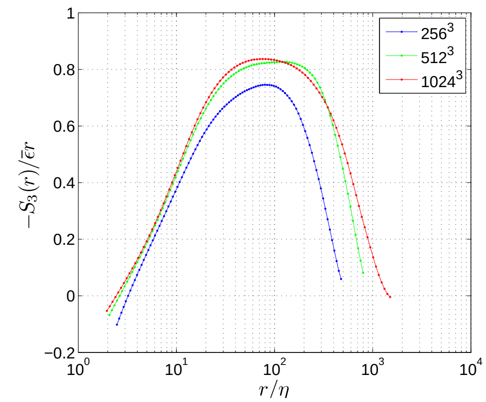

FIG. 1: Scaling of the third-order longtitudal structure function. The value of 4/5 indicates the presence of the inertial range.

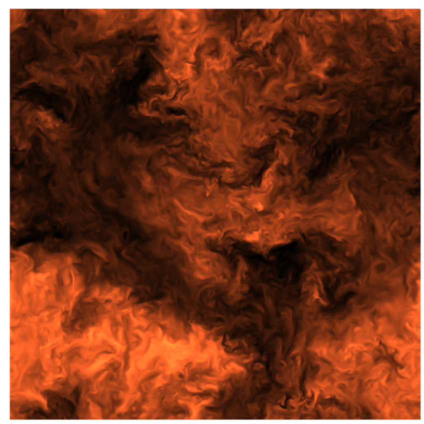

FIG. 2: A velocity component from a 1024^3 run.

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III. DEVELOPMENT OF SGS MODELS

There are four terms that need to be modeled:

- SGS stress $\tau_{ij} = \overline{u_i u_j} - \bar{u}_i \bar{u}_j$;
- SGS scalar flux $\tau_{i\phi} = \overline{u_i \phi} - \bar{u}_i \bar{\phi}$;
- SGS energy dissipation $\epsilon_s = \nu(\overline{\nabla u : \nabla u} - \nabla \bar{u} : \nabla \bar{u})$;
- SGS scalar dissipation $\chi_s = \kappa(\overline{\nabla \phi \cdot \nabla \phi} - \nabla \bar{\phi} \cdot \nabla \bar{\phi})$.

The main research focus is on the understanding the physical properties of the modeled terms through the *a priori* analysis with emphasis on utilization of the tools from statistical geometry. The structure of the small-scale flow features is studied with the help of the DNS database, and the observed statistical conformities are applied in the modeling.

A. SGS stress τ_{ij}

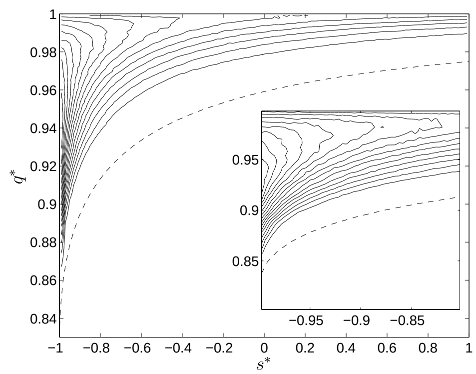

FIG. 3: Joint PDF of (s^*, q^*) as predicted *a priori* from the DNS database.

In the literature the most popular approach for modeling τ_{ij} remains the eddy-viscosity: $\tau_{ij} = \nu_T \bar{S}_{ij}$, where $\bar{S}_{ij}$ is the resolved strain-rate tensor. This approach, although it leads to stable calculations (the net flux of energy from the resolved scales is always positive), suffers from the lack of quality in the prediction of the actual τ_{ij}, which is of great importance in some areas, e.g., modeling of the reacting flows. To evaluate the geometrical structure of τ_{ij} we need two parameters. In [1] two parameters s^* and q^* are introduced in such manner that the measure $ds^*\, dq^*$ is equivalent to the standard measure in the matrix space; this enables us to evaluate various characteristics of τ_{ij} in a turbulent flow using s^* and q^*, such as the most probable stress state or the most popular flow configuration at the smallest scales. Also, these two parameters can be used to evaluate the quality of models encountered in the literature by comparing the distribution of (s^*, q^*) given by the model to the actual distribution computed *a priori* from the data in our database, shown in Figure 3 [1].

Our analysis show that from the most popular classes of models for τ_{ij}, the scale-similarity approach [3] produces the models with the most appropriate joint distribution of s^* and q^* thus giving the most appropriate structure of τ_{ij}.

B. SGS energy dissipation ϵ_s

In the current literature the modeling of ϵ_s is usually dealt with by $\epsilon_s = \frac{k_s^{3/2}}{\Delta}$, where $k_s = \tau_{ii}/2$ is the SGS kinetic energy and Δ is the LES filter size. This model implicitly assumes that the scaling $\epsilon_s \sim k_s^{3/2}$ holds for all values of k_s. Using our DNs database we showed that this assumption holds only in general sense $\epsilon_s \sim k_s^{\gamma}$, where γ is not constant but changes considerably with the filter size Δ, which is shown in Figure 4. See [2] for further details.

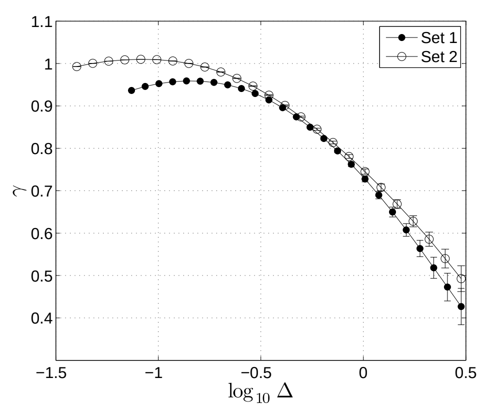

FIG. 4: Scaling of γ with the LES filter width Δ.

[1] S. G. Chumakov. Statistics of subgrid-scale stress states in homogeneous isotropic turbulence. *J. Fluid Mech.*, 562:405–414, 2006.

[2] S. G. Chumakov. Scaling properties of subgrid-scale energy dissipation. *Phys. Fluids*, 2007 (in press).

[3] S. G. Chumakov and C. J. Rutland. Dynamic structure subgrid-scale models for large eddy simulation. *Int. J. Numer. Meth. Fluids*, 47:911–923, 2005.